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Binding energy of the bound polaron in a quantum well within an electric field

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Abstract. The method of a variational wavefunction has been used to study the effect of the electron–LO-phonon interaction on the binding energy of the ground bound state of an isolated hydrogenic impurity in a GaAs–$Ga_{1-x}Al_xAs$ quantum well subjected to an external electric field. The binding energy is obtained as a function of the impurity position z_i, the well width L and the electric field strength F. It was found that the polaronic correction to the impurity binding energy is quite significant. The correction ranges from about 8% when the impurity is placed at the centre to 13–15% when the impurity is placed at the boundary for the thin quantum well.

1. Introduction

Since Bastard (1981) first calculated the donor binding energy in a single quantum well (QW) by using a variational wavefunction, there have been a considerable number of studies concentrating on the bound states associated with hydrogenic impurities in GaAs–$Ga_{1-x}Al_xAs$ QW (Greene and Bajaj 1983, Brum *et al* 1984, Liu and Quinn 1985, Degani and Hipólito 1986, Ercelebi and Süalp 1987).

In addition, the problem of the presence of an external electric field in the QW has also given rise to some more interest in recent years (Mendez *et al* 1982, Bastard *et al* 1983, Brum *et al* 1985, Liu and Cai 1989). When applied along the growth axis, the external electric field changes the QW confinement energies. Mendez *et al* (1982) have observed a sensitive decrease in photoluminescence (PL) signal and a red shift in the PL peak position for increasing field strength F. Bastard *et al* (1983) proposed variational calculations of the eigenstates in an isolated QW structure subjected to an external electric field. Brum *et al* (1985) and Liu and Cai (1989), respectively, calculated the theoretical results of the electric field dependence of the impurity binding energy in a GaAs–$Ga_{1-x}Al_xAs$ QW.

In a number of studies on the electronic properties in a GaAs–$Ga_{1-x}Al_xAs$ QW, although several important aspects of the problems such as the finite barrier and non-parabolicity of the GaAs conduction band have been considered in model calculations, the electron interaction with the optical phonons of GaAs has been ignored. In recent years some workers (Degani and Hipólito 1986, Ercelebi and Süalp 1987) have considered the electron–LO-phonon coupling when determining the binding energy of the

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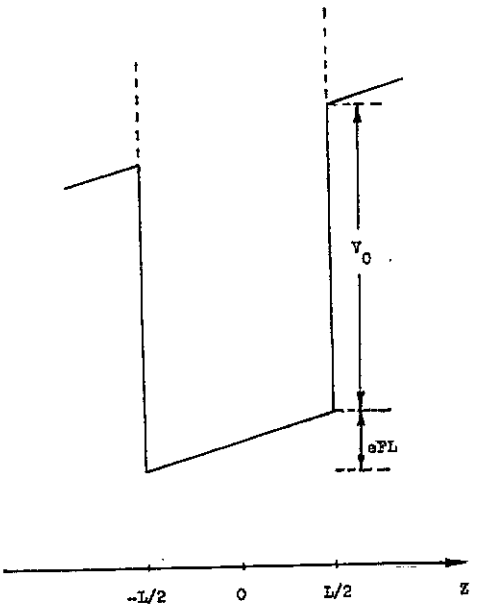

Figure 1. Conduction band profile of a QW subject to an electric field F applied along the growth axis Z.

hydrogenic donor in a QW of infinite barrier in the absence of an external electric field and found that the polaronic contribution to the binding energy is quite significant. However, the polaronic effects have not been considered in an electric field yet.

In this paper, we shall study the effect of the electron–LO-phonon interaction on the binding energy of the ground bound state of an isolated hydrogenic impurity in a QW within an external electric field. By using the variational wavefunction method, we obtain the binding energy of the bound polaron under the adiabatic approximation as a function of the strength of the electric field F, the well width L and the impurity position z_i. The binding energy of the bound polaron may be enhanced or diminished with increasing field strength depending on the impurity location in the QW. We shall show that the effect of the electron–LO-phonon interaction is quite important in increasing the values of binding energies significantly.

2. Theory

Let us consider the bound-state problem associated with a single coulombic impurity located at $z = z_i$ in a GaAs–$Ga_{1-x}Al_xAs$ QW of width L within an external electric field F. The field is assumed to be constant and applied parallel to the growth axis (in the Z direction). As shown in figure 1, we consider the electron to be interacting with the optical phonons of this semiconductor structure. In the effective-mass approximation the Hamiltonian of this system can be written as (Brum *et al* 1985, Degani and Hipólito, 1986)

$$H = \frac{p^2}{2m - e^2} - \frac{e^2}{\varepsilon[x^2 + y^2 + (z - z_i)^2]^{1/2}} + V(z) + |e|Fz + \sum_q \hbar\omega a_q^+ a_q + \sum_q [V_q^* a_q^+ \exp(-i\boldsymbol{q}\cdot\boldsymbol{r}) + \text{HC}] \tag{1}$$

where

$$V_q = \hbar\omega(4\pi\alpha/V_q^2)^{1/2}(\hbar/2m\omega)^{1/4}. \tag{2}$$

The notation is as follows. The electron band mass is m, its position $\boldsymbol{r} = (\boldsymbol{\rho}, z) = (x, y, z)$, and its momentum $\boldsymbol{p}$. The operators a_q^+ and a_q, respectively, create and annihilate a phonon of wavevector $\boldsymbol{q} = (\boldsymbol{Q}, q_z)$ and frequency ω. e stands for the electron charge, and ε is the lattice dielectric constant of the semiconductor structure. The lattice volume is denoted by V and α is the Fröhlich electron–phonon coupling constant. For an infinite QW, $V(z) = 0$ for $-L/2 < z < L/2$ and $V(z) = V_0 \to +\infty$ otherwise.

An exact solution of the Schrödinger equation for the Hamiltonian (1) of the system is not possible. Brum *et al* (1985) have used two approaches, namely a variational approach and an exact approach, to compare the energy-level shifts versus electric field for a conduction electron in a finite GaAs QW. They have observed that the difference is not very great and that in spite of this discrepancy the values of the impurity binding energy appear to be almost independent of the envelope function used. Both the models lead to the same numerical values. Therefore the impurity binding energy can be obtained by the variational envelope function. To obtain the binding energy of the bound polaron in a QW within an electric field, we shall use a variational approach in the following.

In the case of weak coupling and $T \simeq 0$ K, we adopt the well known adiabatic approximation. That is to say, we can choose a simple product wavefunction as the trial wavefunction (Brum *et al* 1985, Degani and Hipólito 1986) for the ground state of the Hamiltonian equation (1), which is given by

$$|\Psi\rangle = \Phi(\boldsymbol{r})U|0\rangle \tag{3}$$

where $|0\rangle$ represents the state with no phonon, i.e. the vacuum state and U is a unitary displacement transformation given by

$$U = \exp\left(\sum_q \frac{V_q\sigma_q(a_q - a_q^+)}{\hbar\omega}\right) \tag{4a}$$

where

$$\sigma_q = \langle\Phi(\boldsymbol{r})|\exp(\pm i\boldsymbol{q}\cdot\boldsymbol{r})|\Phi(\boldsymbol{r})\rangle. \tag{4b}$$

The electron ground-state wavefunction for an infinite QW in an electric field is (Brum *et al* 1985)

$$\Phi(\boldsymbol{r}) = (2/\pi\lambda^2)^{1/2}\varphi(z)\exp(-\rho/\lambda) \tag{4c}$$

with

$$\varphi(z) = \begin{cases} N\cos(\pi z/L)\exp[-\beta(\frac{1}{2} + z/L)] & |z| \leqslant L/2 \\ 0 & |z| > L/2 \end{cases} \tag{4d}$$

where λ and β are two variational parameters and N is a normalization constant given by

$$N = 2\{\beta(\pi^2 + \beta^2)/L[1 - \exp(-2\beta)]\}^{1/2}/\pi. \tag{4e}$$

Using a two-dimensional Fourier expansion of the Coulomb interaction, the expec-

tation value of the Coulomb interaction term is then given by

$$\langle\Psi| - e^2/\varepsilon r|\Psi\rangle = -e^2 f_1(\lambda, \beta)/\varepsilon \tag{5}$$

with

$$f_1(\lambda, \beta) = \int_0^\infty \left[1 + \left(\frac{\lambda Q}{2}\right)^2\right]^{-3/2} \mathrm{d}Q \int_{-L/2}^{L/2} |\varphi(z)|^2 \exp(-Q|z - z_i|)\, \mathrm{d}z. \tag{6}$$

The calculation of the expectation value of H is lengthy. We give here the final result:

$$E(\lambda, \beta) = \langle\Psi|H|\Psi\rangle = \hbar^2/2m\lambda^2 + \hbar^2(\pi^2 + \beta^2)/2mL^2 - e^2 f_1(\lambda, \beta)/\varepsilon$$
$$+ |e|FL(\tfrac{1}{2}\beta + \beta^2/(\pi^2 + \beta^2) - \coth(\beta/2)] - \alpha\hbar\omega f_2(\lambda, \beta) \tag{7}$$

with

$$f_2(\lambda, \beta) = (\hbar/8m\omega)^{1/2} N^2 \exp(-\beta)$$
$$\times \int_0^\infty \frac{\sinh(x + \beta)\, \mathrm{d}x}{(x + \beta)[1 + (\lambda x/L)^2]^{3/2}[1 + (x + \beta)^2/\pi]^2}. \tag{8}$$

The parameters λ and β are determined by minimizing E. Let the solutions of the coupled equations

$$\partial E(\lambda, \beta)/\partial\beta = 0, \tag{9a}$$

and

$$\partial E(\lambda, \beta)/\partial\lambda = 0 \tag{9b}$$

be λ_0 and β_0. We find finally the ground-state energy of the bound polaron in a QW within an electric field:

$$E(\lambda_0, \beta_0) = \hbar^2/2m\lambda_0^2 + \hbar^2(\pi^2 + \beta_0^2)/2mL^2 - e^2 f_1(\lambda_0, \beta_0)/\varepsilon$$
$$+ |e|FL[\tfrac{1}{2}\beta_0 + \beta_0^2/(\pi^2 + \beta_0^2) - \tfrac{1}{2}\coth\beta_0] - \alpha\hbar\omega f_2(\lambda_0, \beta_0). \tag{10}$$

Following Brum *et al* (1985), the bound polaron binding energy is given by

$$E_i = e^2 f_1(\lambda_0, \beta_0)/\varepsilon + \alpha\hbar\omega f_2(\lambda_0, \beta_0) - \hbar^2/2m\lambda_0^2. \tag{11}$$

The second term in (11) is the effect of the electron–LO-phonon interaction on the impurity binding energy. From equations (6), (8) and (11), we have obtained the binding energy $E_i = E_i(L, F, z_i)$ as a function of the well width L, the strength of electric field F and the impurity position z_i along the growth axis.

3. Results and discussion

Equations (9) can only be solved numerically for the values of λ_0 and β_0. Then the above theory is now applied to study the binding energy of bound polaron numerically in a GaAs–$Ga_{1-x}Al_xAs$ QW. We use the following parameters for GaAs: $\varepsilon = 13.1$; $m = 0.0657m_0$, where m_0 is the free-electron mass; $\hbar\omega = 35.2$ meV; $\alpha = 0.0681$.

First we plot the values of the impurity binding energy versus the impurity position along the Z axis for a QW width $L = 80$ Å with several different values of the electric

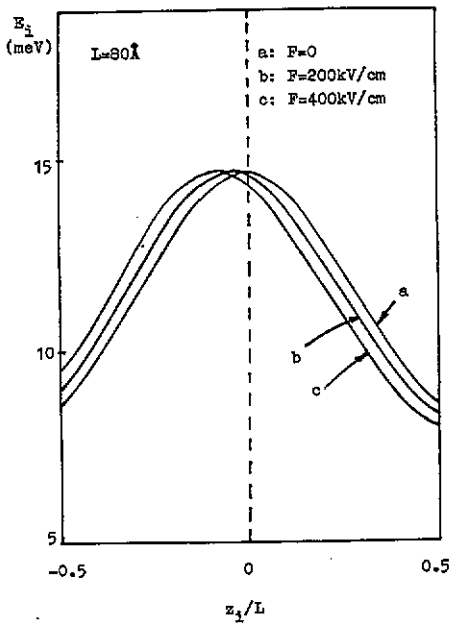

Figure 2. Impurity binding energy as a function of the impurity position along the Z axis for several different values of the electric field F and the well width L = 80 Å.

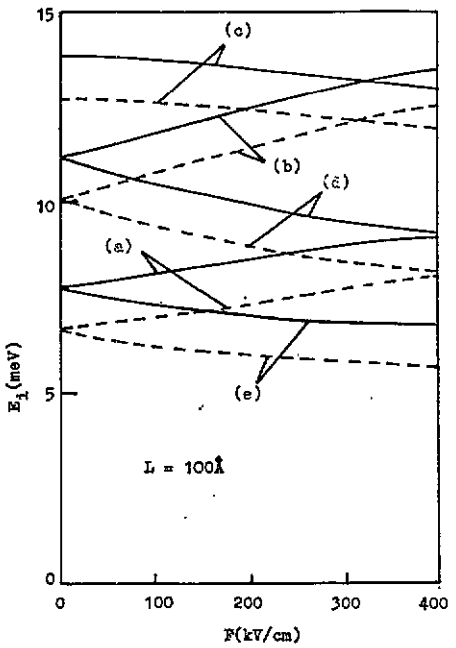

Figure 3. Impurity binding energy as a function of the electric field for the well width L = 100 Å: ——, with the electron–LO-phonon interaction; – – –, without the electron–LO-phonon interaction. Five impurity positions are considered: curves (a) $-L/2$; curves (b) $-L/4$; curves (c) 0; curves (d) $L/4$; curves (e) $L/2$.

field: $F = 0$, 200 kV cm^{-1} and 400 kV cm^{-1}, as shown in figure 2. We observe that the binding energy decreases as the impurity moves from the centre to the edge of the well. This is because the repulsive barrier potential tends to push the electronic charge distributions away from the donor and leads to a reduced Coulomb attraction. When the impurity is placed at $z_i \geqslant 0$, the binding energy decreases with increasing field strength but, when the impurity is at $z_i < 0$, the binding energy increases with increasing F. We can also observe that the impurity binding energy has a maximum at $z_i = 0$ for $F = 0$ and the impurity position of maximum binding energy has a small negative shift from the centre of the well with increasing strength of the electric field. All these are associated with the electric-field-induced deformation of the wavefunction of the electron. The electron wavefunction tends to concentrate near the interface $z = -L/2$ in the presence of the electric field.

Let us calculate the effect of the electron–LO-phonon coupling on the impurity binding energy. We have obtained the results by numerically minimizing the energy expression equation (7), with and without the electron–LO-phonon interaction for a QW when its width L = 100 Å and when there are several different positions of the donor: $z_i = -L/2$, $-L/4$, 0, $L/4$ and $L/2$. The binding energy is plotted as a function of the electric field as shown in figure 3. The full and broken curves represent the system with and without the electron–LO-phonon interaction, respectively. The percentage effects on the impurity binding energy due to the electron–LO-phonon interaction for several values of the electric field F and different impurity positions z_i and the well width L_1 =

Table 1. Percentage effects on the impurity binding energy, $\Delta E_i = [(E_i - E_i^*)/E_i] \times 100\%$, where E_i and E_i^* are the binding energies with and without the electron–LO-phonon coupling, respectively, for several values of the electric field F and different impurity positions z_i. The well width $L_1 = 40$ Å or $L_2 = 100$ Å.

	$F = 0$ kV cm^{-1}		$F = 50$ kV cm^{-1}		$F = 100$ kV cm^{-1}		$F = 150$ kV cm^{-1}		$F = 200$ kV cm^{-1}	
z_i/L	L_1	L_2	L_1	L_2	L_1	L_2	L_1	L_2	L_1	L_2
−0.5	13.1	14.7	13.1	14.3	13.0	14.0	13.0	13.5	13.0	13.1
0	8.8	8.3	8.8	8.3	8.8	8.2	8.8	8.2	8.8	8.2
0.5	13.1	14.7	13.1	14.9	13.1	15.2	13.1	15.4	13.2	15.5

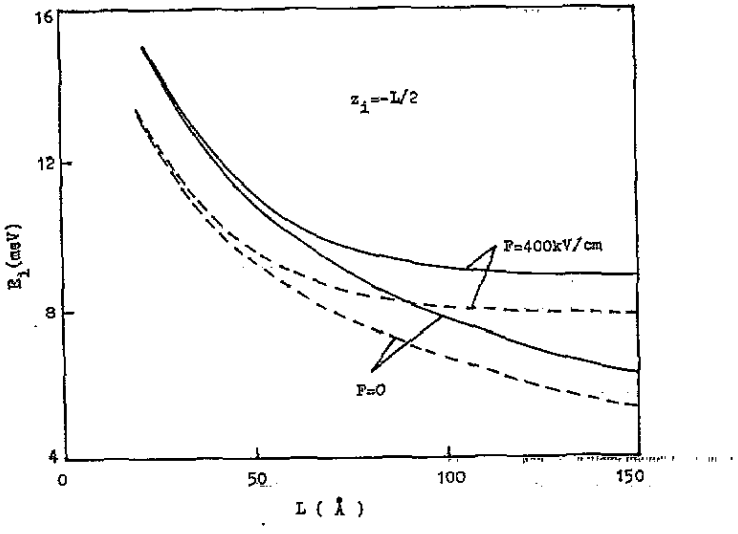

Figure 4. Impurity binding energy as a function of the well width for the impurity position $z_i = -L/2$: ——, with the electron–LO-phonon interaction; – – –, without the electron–LO-phonon coupling. Two values of the electric field are considered: $F = 0$ and 400 kV cm^{-1}.

40 Å or $L_2 = 100$ Å are also given in table 1. It is found that the effect of the electron–LO-phonon coupling is quite important in increasing the values of the impurity binding energy significantly. We can see that for a given well width the polaronic correction to the binding energy decreases with increasing electric field when the impurity is placed at $z_i < 0$, and the situation is reversed when the impurity is located at $z_i > 0$. We can also note that for a given F when the impurity is placed at the centre of the QW the polaronic contribution is greater for a smaller well width. However, when the impurity is located at the boundary of the barrier, the electron–LO-phonon interaction effect on the binding energy becomes smaller for smaller well thicknesses. These results are similar to the results obtained without an electric field by Degani and Hipólito (1986).

In figure 4, we also calculate the impurity binding energy as a function of the well width when the values of the electric field are $F = 0$ or $F = 400$ kV cm^{-1} and the impurity position is $z_i = -L/2$. The full and broken curves correspond to the cases with and

without electron–LO-phonon coupling, respectively. The result that the curves flatten at large enough L if F is non-zero is identical with the result of Brum *et al* (1985).

In conclusion, we have studied the effect of the electron–LO-phonon coupling on the binding energy of the ground bound state of an isolated hydrogenic impurity in a QW within an electric field by using the variational wavefunction method. We have obtained the binding energy of the bound polaron as a function of the electric field intensity F, the well thickness L and the impurity position z_i. The binding energy may be enhanced or diminished with increasing field intensity depending on the impurity location in the QW. Our computations show that the electron–LO-phonon interaction causes a significant correction to the impurity binding energy. This correction ranges from about 8% when the impurity is placed at the centre ($z_i = 0$) to 13–15% when the impurity is located at the boundary ($z_i = \pm L/2$) for $L = 40$ Å and 100 Å and $F = 0$ and 200 kV cm^{-1}. This correction range is fundamentally the same as the result which was obtained at a low electronic density in the absence of an electric field by Degani and Hipólito (1986).

Furthermore, we would like to say a word on the influence of the surface optical (SO) phonons on the impurity binding energy. It is reasonable to consider such an influence if we wish to obtain a more detailed polaronic correction. However, a basic conclusion which has been drawn for a polaron in a single heterostructure within a magnetic field by one of the present authors and co-workers (Chen *et al* 1987a, b) and for a polaron in a double heterostructure by Lin *et al* (1991) showed that the energy correction due to SO-phonon contribution amount is smaller than that due to the LO-phonon contribution when the well width is not sufficiently narrow. So as a consequence the influence of the LO phonons on the polaronic correction for the impurity binding energy prevails.

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